

Safety Data Sheet

Diepoxybutane

Division of Safety
National Institutes
of Health



WARNING!

THIS COMPOUND IS ABSORBED THROUGH THE SKIN AND THE RESPIRATORY TRACT. IT IS TOXIC, CARCINOGENIC, AND MUTAGENIC AND MAY IRRITATE TISSUES. AVOID FORMATION AND BREATHING OF AEROSOLS OR VAPORS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, DRINK PLENTY OF WATER OR MILK. INDUCE VOMITING. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF AEROSOLS OR VAPORS. USE WATER TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

A. Background

Diepoxybutane (DEB) is a colorless reactive liquid. It is absorbed through the skin and the respiratory tract. It is a severe irritant to lungs, skin, and eyes and is toxic to humans and animals by all routes. As an alkylating agent, it is carcinogenic in rodents and mutagenic to lower species and to animal cells in vitro. DEB is used commercially in the preparation of erythritol and other pharmaceuticals, as a cross-linking agent for textile fibers, and in polymer curing; in the laboratory it serves as a theoretical model in studies of carcinogens.

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...having two asymmetric carbon atoms, exists in four forms: D, L, DL, and meso. These forms differ in some of their chemical, physical, and toxicological properties.

B. Chemical and Physical Data

1. Chemical Abstract No.: 1464-53-5(mixture)

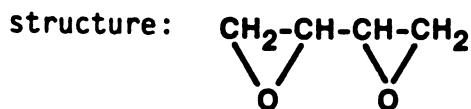
2. Synonyms:

DEB	Butadiene dioxide
1,1'-Bi(ethylene) oxide	2,4-Diepoxybutane
Bioxiran	1,2:3,4-Diepoxybutane
Bioxirane	Dioxybutadiene
2,2'-Bioxirane (9CI)	Erythritol anhydride
Butanedione	1,2:3,4-Dianhydro-threitol
Butadiene diepoxide	

Other forms:

DL-Diepoxybutane	C.A. 298-18-0
(+ -)-2,2'-Bioxirane	(+ -)-1,2:3,4-Diepoxybutane
dl-Butadiene dioxide	DL-1,2:3,4-Diepoxybutane
1,2:3,4-Dianhydro-DL-threitol	(R*,R*)-(+ -)-2,2'-Bioxirane
dl-1,2:3,4-Diepoxybutane	
L-Diepoxybutane	C.A. 30031-64-2
L-Butadiene diepoxide	L-1,2:3,4-Diepoxybutane
(S-(R*,R*)) -2,2'-Bioxirane	(2S,3S)-1,2:3,4-Diepoxybutane
(2S,3S)-Diepoxybutane	NSC-32606
meso-Diepoxybutane	C.A. 564-00-1
(R*,S*)-2,2'-Bioxirane	Erythritol anhydride
1,2:3,4-Dianhydroerythritol	
meso-1,2,3,4-Diepoxybutane	
(R*,S*)-Diepoxybutane	

3. Molecular
formula:
 $C_4H_6O_2$
weight:
86.1



4. Density: 1.113 g/cm^3 at 18°C relative to water at 4°C .
5. Absorption spectroscopy: IR epoxide band at 2150 cm^{-1} .
6. Volatility: 3.9 mm Hg at 20°C .
7. Solubility: Miscible with water and ethanol.
8. Description, appearance: Colorless liquid.
9. Boiling point: 138°C (mixture); $140\text{--}142^\circ\text{C}$ (meso); 144°C (DL).
Melting point: -19°C (meso); 4°C (DL).
10. Stability: Hydrolyzes slowly in water, faster in the presence of acid or base.
11. Chemical reactivity: Highly reactive because of the ease of opening the three-membered rings. Reacts with alcohols, amines, phenols, and other reactive substances.
12. Flash point: No data.
13. Autoignition temperature: No data.
14. Explosive limits in air: No data.

Fire, Explosion, and Reactivity Hazard Data

1. DEB does not require special fire-fighting procedures or equipment and does not present unusual fire and explosion hazards.
2. Unstable in presence of acids and bases.
3. There are no hazardous decomposition products.
4. Nonspark equipment is not required.

Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving DEB.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by DEB or the materials used for cleanup. If more than 10 ml has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Wash surfaces with copious quantities of water. Glassware should be rinsed (in a hood) with ethanol, followed by soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing DEB shall be disposed of in sinks or general refuse. Surplus DEB or chemical waste streams contaminated with DEB shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (e.g., animal carcasses and bedding) containing DEB shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (e.g., tissue cultures) containing DEB shall be packaged for incineration, as above. Burnable waste (e.g., absorbent bench top liners) minimally contaminated with DEB shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (e.g., associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing DEB shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store in sealed containers under refrigeration (freezer preferred).

Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

1. Sampling: No field methods have been described.
2. Separation and analysis: Various chromatographic (Fishbein and Falk, 1969) and spectrometric (Jungnickel et al., 1953) procedures for the analysis of epoxides have been reviewed. A spectrophotometric method for the analysis of nanomole quantities of epoxides in water has been reported (Mishmash and Meloen, 1972).

Biological Effects (Animal and Human)

1. Absorption: DEB is readily absorbed through the skin and the respiratory tract. Absorption through ingestion is questionable, except perhaps at very high doses, since small quantities are hydrolyzed in the gastrointestinal tract. While DEB produces topical irritation in the eyes, there is no evidence whether it is absorbed parenterally by this route.

2. Distribution: Distributed to the lungs after intraperitoneal injection, to thymus and spleen after inhalation, and to the hematopoietic and lymphatic systems after intramuscular injection.
3. Metabolism and excretion: There are no data concerning the metabolism of DEB. However, by analogy with the metabolism of other epoxides, one may assume two reactions: (a) hydrolysis (detoxification) to erythritol and threitol and (b) alkylation of nucleophiles such as alcohols, amino, and thiol groups of tissue constituents. These reactions, plus a reported covalent linkage to DNA, may be related to the carcinogenic action of DEB. There are no data concerning excretory products.
4. Toxic effects: Acute LD50s in mammals are in the range of 25 mg/kg by injection, 90-800 mg/kg through skin, 80-200 mg/kg by the oral route, and 55-90 mg/kg by inhalation. While there are not enough data for a comparison of the various isomers of DEB in the same species by the same route, it appears that the meso form is more toxic than the DL or L form.
5. Carcinogenic effects: DEB produces skin tumors in mice when applied to the skin, local fibrosarcomas at the (subcutaneous) injection site in mice and rats, and lung tumors in mice after intraperitoneal administration.
6. Mutagenic and teratogenic effects: DEB is mutagenic to several strains of plants, bacteria, and Drosophila and to rat and hamster cells in vitro, but not to mice. There are no data on teratogenicity.

Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water or milk. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician. Consider treatment for pulmonary irritation.

References

Fishbein, L., and H. Falk. 1969. Chromatography of alkylating agents. Chrom Rev 11:365-455.

Jungnickel, J.L., E.D. Peters, A. Polgar, and F.T. Weiss. 1953.

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